Condensed phase of converting boson-fermion mixtures

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Theory of a condensed state of hybridised bosons and fermions is developed. Normal and anomalous Green's functions are obtained diagrammatically and analytically using the Hamiltonian of the boson-fermion model (BFM). A pairing of bosons analogous to the Cooper pairing of fermions is found. There are three coupled condensates in the model, described by the off-diagonal single-particle boson, pair-fermion and pair-boson fields. The Gor'kov expansion in the strength of the order parameter near the transition yields no linear homogeneous term in the Ginzburg-Landau equation, and the *infinite* Levanyuk-Ginzburg parameter, $Gi = \infty$, which indicates that previous mean-field discussions of BFM are flawed.

A two component model of negative U centers coupled with the Fermi sea of itinerant fermions was originally employed to study superconductivity in disordered metal-semiconductor alloys [1, 2]. Later on it was applied more generally to describe pairing electron processes with localisation-delocalisation [3], and to the polaron-bipolaron crossover problem in the intermediate electron-phonon coupling regime [4]. The model attracted more attention in connection with exotic [5], and high-temperature superconductors [6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18]. When the attractive potential U is large, the model is reduced to localised bosons spontaneously decaying into itinerant electrons and vice versa, different from a non-converting mixture of mobile charged bosons and fermions [19, 20]. More recently this boson-fermion model has been adopted for a description of superfluidity of atomic fermions scattered into bound (molecular) states [21].

Most studies of BFM below its transition into a low-temperature condensed phase applied a mean-field approximation (MFA), replacing zero-momentum boson operators by c-numbers and neglecting the boson self-energy in the density sum rule [5, 7, 8, 10, 11, 17, 18, 21]. When the bare boson energy is well above the chemical potential, the BCS ground state was found with bosons being only virtually excited [7, 8]. MFA led to a conclusion that BFM exhibits features compatible with BCS characteristics [10], and describes a crossover from the BCS-like to local pair behaviour [18]. The transition was found more mean-field-like than the usual Bose condensation, i.e. characterized by a relatively small value of Gi [11].

At the same time our study of BFM [12] beyond MFA revealed a crucial effect of the boson self-energy on the normal state boson spectral function and the transition temperature T_c. Ref.[12] proved that the Cooper pairing of fermions via virtual bosonic states is impossible in any-dimensional BFM. It occurs only simultaneously with the Bose-Einstein condensation of real bosons in 3D BFM [13, 14], and vanishes in 2D BFM due to the absence of the Bose-Einstein condensation in two dimensions [13]. The origin of this simultaneous condensation lies in a softening of the boson mode at $T = T_c$ caused by its hy-

bridization with fermions. The energy of zero-momentum bosons is renormalized down to *zero* at $T = T_c$, no matter how weak the boson-fermion coupling and how large the bare boson energy are. Bosons look like overdamped diffusive modes, rather than quasiparticles in the long-wave limit [12, 13, 15] contrary to the conclusion of Ref.[9] that there is 'the onset of coherent free-particle-like motion of the bosons' in this limit. One can expect that the boson self-energy should qualitatively modify the whole condensed phase of 3D BFM below T_c.

In this Letter a closed set of equations for fermion and boson Green's functions (GFs) is derived taking into account self-energy effects in the condensed state of 3D BFM. There exist a boson *pair* condensate along with the fermion Cooper pair and the single-particle boson condensate in the model. Remarkably, the Gor'kov expansion [22] of GFs in the strength of the order parameter yields a zero linear term at *any* temperature below T_c, and $Gi = \infty$. It shows that the transition is not a mean-field second order transition, and there is no crossover from the BCS-like to a local pair behaviour at any values of the parameters of BFM.

The Hamiltonian of BFM in an external magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$ is defined as

$$
\begin{aligned}
H &= \int d\mathbf{r} \sum_s \psi_s^\dagger(\mathbf{r}) \hat{h}(\mathbf{r}) \psi_s(\mathbf{r}) + g[\phi(\mathbf{r}) \psi_\uparrow^\dagger(\mathbf{r}) \psi_\downarrow^\dagger(\mathbf{r}) + H.c.] \\
&+ E_0 \phi^\dagger(\mathbf{r}) \phi(\mathbf{r}),
\end{aligned} \tag{1}
$$

where $\psi_s(\mathbf{r})$ and $\phi(\mathbf{r})$ are fermionic and bosonic fields, $s = \uparrow, \downarrow$ is the spin, E_0 is the bare energy of bosons with respect to their chemical potential 2μ, $\hat{h}(\mathbf{r}) = -\left[\nabla + ie\mathbf{A}(\mathbf{r})\right]^2/(2m) - \mu$ is the fermion kinetic energy operator, and g is the hybridization interaction converting a boson into two fermions and vice versa. Here and further I take $\hbar = c = k_B = 1$, and the volume of the system $V = 1$.

The Matsubara field operators, $Q = \exp(H\tau) Q(\mathbf{r}) \exp(-H\tau)$, $\bar{Q} = \exp(H\tau) Q^\dagger(\mathbf{r}) \exp(-H\tau)$ ($Q \equiv \psi_s, \phi$) evolve with the imaginary time $-1/T \leqslant \tau \leqslant 1/T$ as

$$-\frac{\partial \psi_\uparrow(\mathbf{r},\tau)}{\partial \tau} = \hat{h}(\mathbf{r})\psi_\uparrow(\mathbf{r},\tau) + g\phi(\mathbf{r},\tau)\bar{\psi}_\downarrow(\mathbf{r},\tau), \quad (2)$$

$$\frac{\partial \bar{\psi}_\downarrow(\mathbf{r},\tau)}{\partial \tau} = \hat{h}^*(\mathbf{r})\bar{\psi}_\downarrow(\mathbf{r},\tau) - g\bar{\phi}(\mathbf{r},\tau)\psi_\uparrow(\mathbf{r},\tau), \quad (3)$$

$$-\frac{\partial \phi(\mathbf{r},\tau)}{\partial \tau} = E_0\phi(\mathbf{r},\tau) + g\psi_\downarrow(\mathbf{r},\tau)\psi_\uparrow(\mathbf{r},\tau). \quad (4)$$

The theory of the condensed state can be formulated with the normal and anomalous fermion GFs [22], $\mathcal{G}(\mathbf{r},\mathbf{r}',\tau) = -\langle T_\tau \psi_s(\mathbf{r},\tau)\bar{\psi}_s(\mathbf{r}',0)\rangle$, $\mathcal{F}^+(\mathbf{r},\mathbf{r}',\tau) = \langle T_\tau \bar{\psi}_\downarrow(\mathbf{r},\tau)\bar{\psi}_\uparrow(\mathbf{r}',0)\rangle$, respectively, where the operation T_τ performs the time ordering. Fermionic and bosonic fields condense simalteneously [12]. Following Bogoliubov [23] the bosonic condensate is described by separating a large matrix element $\phi_0(\mathbf{r})$ in $\phi(\mathbf{r},\tau)$ as a number, while the remaining part $\tilde{\phi}(\mathbf{r},\tau)$ describes a supracondensate field, $\phi(\mathbf{r},\tau) = \phi_0(\mathbf{r}) + \tilde{\phi}(\mathbf{r},\tau)$. Then using Eq.(4) one obtains

$$g\phi_0(\mathbf{r}) = \Delta(\mathbf{r}) \equiv -\frac{g^2}{E_0}\mathcal{F}(\mathbf{r},\mathbf{r},0+), \quad (5)$$

where $\mathcal{F}(\mathbf{r},\mathbf{r}',\tau) = \langle T_\tau \psi_\downarrow(\mathbf{r},\tau)\psi_\uparrow(\mathbf{r}',0)\rangle$. The equations for GFs are obtained by using Eqs (2,3,4) and the diagrammatic technique [24] in the framework of the noncrossing approximation [25], as shown in Fig.1 and Fig.2.

An important novel feature of BFM is a pairing of supracondensate bosons, generated by their hybridization with the fermionic condensate, as follows from the last diagram in Fig.2. Hence, one has to introduce an *anomalous* supracondensate boson GF, $\mathcal{B}^+(\mathbf{r},\mathbf{r}',\tau) = \langle T_\tau \tilde{\bar{\phi}}(\mathbf{r},\tau)\tilde{\bar{\phi}}(\mathbf{r}',0)\rangle$ along with a normal boson GF, $\mathcal{D}(\mathbf{r},\mathbf{r}',\tau) = -\langle T_\tau \tilde{\phi}(\mathbf{r},\tau)\tilde{\bar{\phi}}(\mathbf{r}',0)\rangle$. The diagrams, Fig.1 and Fig.2, are transformed into analytical equations for time Fourier-components of the fermion GFs with the Matsubara frequencies $\omega = \pi T(2n+1)$ $(n = 0, \pm 1, \pm 2, ...)$ as

$$[i\omega - \hat{h}(\mathbf{r})]\mathcal{G}_\omega(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') - \Delta(\mathbf{r})\mathcal{F}_\omega^+(\mathbf{r},\mathbf{r}')$$
$$- g^2 T \sum_{\omega'}\int d\mathbf{x} \mathcal{G}_{-\omega'}(\mathbf{x},\mathbf{r})\mathcal{D}_{\omega-\omega'}(\mathbf{r},\mathbf{x})\mathcal{G}_\omega(\mathbf{x},\mathbf{r}')$$
$$- g^2 T \sum_{\omega'}\int d\mathbf{x} \mathcal{F}_{\omega'}^+(\mathbf{r},\mathbf{x})\mathcal{B}_{\omega+\omega'}(\mathbf{r},\mathbf{x})\mathcal{F}_\omega^+(\mathbf{x},\mathbf{r}'), \quad (6)$$

$$[-i\omega - \hat{h}^*(\mathbf{r})]\mathcal{F}_\omega^+(\mathbf{r},\mathbf{r}') = \Delta^*(\mathbf{r})\mathcal{G}_\omega(\mathbf{r},\mathbf{r}')$$
$$- g^2 T \sum_{\omega'}\int d\mathbf{x} \mathcal{G}_{\omega'}(\mathbf{r},\mathbf{x})\mathcal{D}_{\omega'-\omega}(\mathbf{x},\mathbf{r})\mathcal{F}_\omega^+(\mathbf{x},\mathbf{r}')$$
$$+ g^2 T \sum_{\omega'}\int d\mathbf{x} \mathcal{F}_{-\omega'}(\mathbf{r},\mathbf{x})\mathcal{B}_{-\omega-\omega'}^+(\mathbf{r},\mathbf{x})\mathcal{G}_\omega(\mathbf{x},\mathbf{r}') \quad (7)$$

and,

$$(i\Omega - E_0)\mathcal{D}_\Omega(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')$$
$$- g^2 T \sum_{\omega'}\int d\mathbf{x} \mathcal{G}_{\omega'}(\mathbf{r},\mathbf{x})\mathcal{G}_{\Omega-\omega'}(\mathbf{r},\mathbf{x})\mathcal{D}_\Omega(\mathbf{x},\mathbf{r}')$$
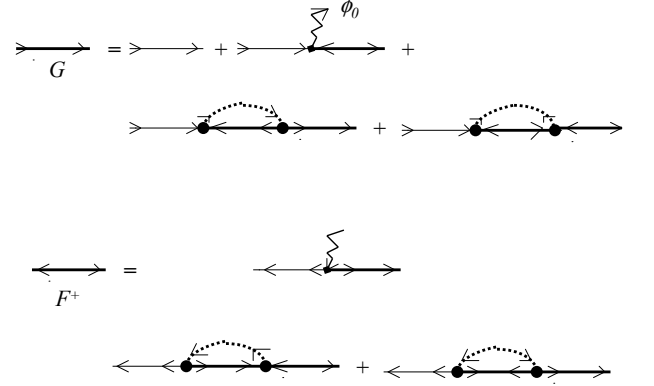

FIG. 1: Diagrams for the normal and anomalous fermion GFs. Vertexes (dots) correspond to the hybridization interaction g, and zig-zag arrows represent the single-particle Bose condensate ϕ_0.

$$- g^2 T \sum_{\omega'}\int d\mathbf{x} \mathcal{F}_{\omega'}(\mathbf{r},\mathbf{x})\mathcal{F}_{\Omega-\omega'}(\mathbf{r},\mathbf{x})\mathcal{B}_\Omega^+(\mathbf{x},\mathbf{r}'), \quad (8)$$

$$(-i\Omega - E_0)\mathcal{B}_\Omega^+(\mathbf{r},\mathbf{r}') =$$
$$g^2 T \sum_{\omega'}\int d\mathbf{x} \mathcal{F}_{-\omega'}^+(\mathbf{r},\mathbf{x})\mathcal{F}_{-\Omega+\omega'}^+(\mathbf{r},\mathbf{x})\mathcal{D}_\Omega(\mathbf{x},\mathbf{r}')$$
$$- g^2 T \sum_{\omega'}\int d\mathbf{x} \mathcal{G}_{-\omega'}(\mathbf{x},\mathbf{r})\mathcal{G}_{\omega'-\Omega}(\mathbf{x},\mathbf{r})\mathcal{B}_\Omega^+(\mathbf{x},\mathbf{r}'). \quad (9)$$

for the boson GFs with $\Omega = 2\pi T n$, and $\mathcal{B}(\mathbf{r},\mathbf{r}',\tau) = \langle T_\tau \tilde{\phi}(\mathbf{r},\tau)\tilde{\phi}(\mathbf{r}',0)\rangle$

These equations can be formally solved in the homogeneous case without the external field, $\mathbf{A} = 0$. Transforming into the momentum space yields GFs' time-space Fourier components as

$$\mathcal{G}(\mathbf{k},\omega) = -\frac{i\tilde{\omega}^* + \xi_\mathbf{k}}{|i\tilde{\omega} - \xi_\mathbf{k}|^2 + |\tilde{\Delta}(\mathbf{k},\omega)|^2}, \quad (10)$$

$$\mathcal{F}^+(\mathbf{k},\omega) = \frac{\tilde{\Delta}^*(\mathbf{k},\omega)}{|i\tilde{\omega} - \xi_\mathbf{k}|^2 + |\tilde{\Delta}(\mathbf{k},\omega)|^2}, \quad (11)$$

and

$$\mathcal{D}(\mathbf{q},\omega) = -\frac{i\tilde{\Omega}^* + E_0}{|i\tilde{\Omega} - E_0|^2 + |\Gamma(\mathbf{q},\Omega)|^2}, \quad (12)$$

$$\mathcal{B}^+(\mathbf{q},\omega) = \frac{\Gamma^*(\mathbf{q},\Omega)}{|i\tilde{\Omega} - E_0|^2 + |\Gamma(\mathbf{q},\Omega)|^2}, \quad (13)$$

where $\tilde{\omega} \equiv \omega + i\Sigma_f(\mathbf{k},\omega)$, $\tilde{\Omega} \equiv \Omega + i\Sigma_b(\mathbf{q},\Omega)$. The fermionic order parameter, renormalised with respect to
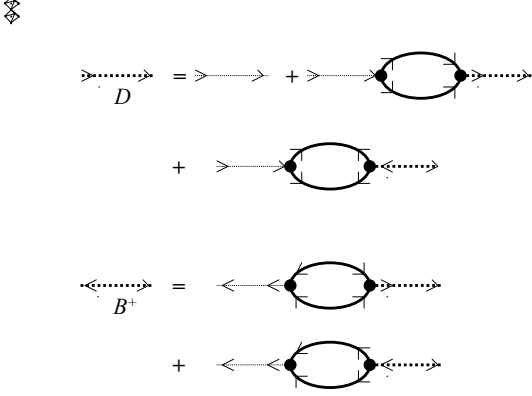
FIG. 2: Diagrams for the supracondensate boson GFs. The Cooper-pairing of fermions leads to the Cooper-pair-like boson condensate, described by the boson anomalous GF, $\mathcal{B}^+$.

the mean-field Δ due to the formation of the boson-pair condensate, is given by

$$\tilde{\Delta}(\mathbf{k}, \omega) = \Delta + g^2 T \sum_{\omega'} \int \frac{d\mathbf{q}}{2\pi^3} \mathcal{F}^+(\mathbf{k} - \mathbf{q}, \omega') \mathcal{B}(\mathbf{q}, \omega + \omega'),$$
(14)

and the boson-pair order parameter, generated by the hybridization with the fermion Cooper pairs, is

$$\Gamma(\mathbf{q}, \Omega) = g^2 T \sum_{\omega'} \int \frac{d\mathbf{k}}{2\pi^3} \mathcal{F}(\mathbf{k}, \omega') \mathcal{F}(\mathbf{q} - \mathbf{k}, \Omega - \omega'). \quad (15)$$

Hence, there are three coupled condensates in the model described by the off-diagonal fields $g\phi_0$, $\tilde{\Delta}$, and Γ, rather than two, as in MFA. At low temperatures all of them have about the same magnitude, as the fermion and boson self-energies,

$$\Sigma_f(\mathbf{k}, \omega) = -g^2 T \sum_{\omega'} \int \frac{d\mathbf{q}}{2\pi^3} \mathcal{G}(\mathbf{q} - \mathbf{k}, -\omega') \mathcal{D}(\mathbf{q}, \omega - \omega'),$$
(16)

$$\Sigma_b(\mathbf{q}, \Omega) = -g^2 T \sum_{\omega'} \int \frac{d\mathbf{q}}{2\pi^3} \mathcal{G}(\mathbf{k}, \omega') \mathcal{G}(\mathbf{q} - \mathbf{k}, \Omega - \omega'),$$
(17)

respectively.

On the other hand, when the temperature is close to T_c (i.e. $T_c - T \ll T_c$), the boson pair condensate is weak compared with the single-particle boson and the Cooper pair condensates. Since Γ, Eq.(15) is of the second order in Δ, $\Gamma \propto \Delta^2$, the anomalous boson GF can be neglected in this temperature range, where Δ is small. The fermion self-energy, Eq.(16) is a regular function of

ω and $\mathbf{k}$, so that it can be absorbed in the renormalized fermion band dispersion. Then the fermion normal and anomalous GFs, Eqs.(10,11) look like the familiar GFs of the BCS theory, and one can apply the Gor'kov expansion [22] in powers of $\Delta(\mathbf{r})$ to describe the condensed phase of BFM in the magnetic field near the transition. Using Eq.(7) and Eq.(5) one obtains to the terms linear in Δ

$$\Delta^*(\mathbf{r}) = \frac{g^2}{E_0} T \sum_{\omega_n} \int d\mathbf{x} \, \mathcal{G}^{(n)}_{-\omega_n}(\mathbf{x}, \mathbf{r}) \Delta^*(\mathbf{x}) \mathcal{G}^{(n)}_{\omega_n}(\mathbf{x}, \mathbf{r}). \quad (18)$$

The spatial variations of the vector potential are small near the transition. If $\mathbf{A}(\mathbf{r})$ varies slowly, the normal state GF, $\mathcal{G}^{(n)}_\omega(\mathbf{r}, \mathbf{r}')$ differs from the zero-field normal state GF, $\mathcal{G}^{(0)}_\omega(\mathbf{r} - \mathbf{r}')$ only by a phase [22] $\mathcal{G}^{(n)}_\omega(\mathbf{r}, \mathbf{r}') = \exp[-ie\mathbf{A}(\mathbf{r}) \cdot (\mathbf{r} - \mathbf{r}')] \mathcal{G}^{(0)}_\omega(\mathbf{r} - \mathbf{r}')$. Expanding all quantities near the point $\mathbf{x} = \mathbf{r}$ in Eq.(18) up to the second order in $\mathbf{x} - \mathbf{r}$ inclusive, one obtains the linearised equation for the fermionic order parameter as

$$\gamma[\nabla - 2ie\mathbf{A}(\mathbf{r})]^2 \Delta(\mathbf{r}) = \alpha \Delta(\mathbf{r}), \quad (19)$$

where

$$\alpha = 1 + \frac{\Sigma_b(0,0)}{E_0} \approx 1 - \frac{g^2 N(0)}{E_0} \ln \frac{\mu}{T}, \quad (20)$$

and $\gamma \approx 7\zeta(3) v_F^2 g^2 N(0)/(48\pi^2 T^2 E_0)$. Here v_F is the Fermi velocity, and $N(0)$ is the (renormalized) fermion density of states at the Fermi level.

In the framework of MFA one takes the bare boson energy in Eq.(20) as a temperature independent parameter, $E_0 = g^2 N(0) \ln(\mu/T_c)$ [11], or determines it from the conservation of the total number of particles (the density sum-rule) neglecting the boson self-energy $\Sigma_b(\mathbf{q}, \Omega)$ [8, 17, 18, 21]). Then Eq.(19) looks like the conventional mean-field Ginzburg-Landau (GL) equation with a negative $\alpha \propto T - T_c$, a relatively small fluctuation region Gi [11], and a finite $H_{c2}(T)$ [17]. As a result one concludes that the phase transition is almost the conventional BCS-like transition, at least at $E_0 \gg T_c$ [7, 11], and BFM, Eq.(1) describes the crossover from the BCS-like to local pair behaviour by tuning the parameters [18]. This conclusion is incorrect. The main problem with MFA stems from the density sum-rule, which determines the chemical potential of the system and consequently the bare boson energy $E_0(T)$ as a function of temperature,

$$-T \sum_{\Omega_n} e^{i\Omega_n \tau} \int \frac{d\mathbf{q}}{2\pi^3} D(\mathbf{q}, \Omega_n) = n_b - \int d\mathbf{r} |\phi_0(\mathbf{r})|^2. \quad (21)$$

Here $\tau = +0$, $n_b = n - n_f$ is the number of bosons, n is the total number of particles, and n_f is the number of fermions. The term of the sum in Eq.(21) with $\Omega_n = 0$ is given by the integral

$$T \int \frac{d\mathbf{q}}{2\pi^3} \frac{1}{E_0 + \Sigma_b(\mathbf{q}, 0)}, \quad (22)$$

where $\Sigma_b(\mathbf{q}, 0) = \Sigma_b(0,0) + q^2/2M^*$ for a small $\mathbf{q}$ is calculated using Eq.(17) with the normal state fermion GF [12] (here M^* is a constant). The integral converges, if and only if $E_0 \geqslant -\Sigma_b(0,0)$. This exact result means that $\alpha \geqslant 0$ at any temperature. In fact, this coefficient is strictly zero in the Bose-condensed state, because $\mu_b = -[E_0 + \Sigma_b(0,0)]$ corresponds to the boson chemical potential relative to the lower edge of the boson energy spectrum. More generally, $\mu_b = 0$ corresponds to the appearance of the Goldstone-Bogoliubov mode due to a broken symmetry below T_c. As a result, the GL coefficient $\alpha(T)$, is *zero* at *any* temperature below T_c, $\alpha(T) \equiv 0$, and not only at T_c in the exact theory of BFM. On the other hand, MFA violates the density sum-rule, predicting the wrong negative $\alpha(T)$ below T_c.

There are a few important physical consequences. Since $\alpha(T) = 0$, the Levanyuk-Ginzburg parameter [26] is infinite. It means that the phase transition is never a BCS-like second-order phase transition even at large E_0 and small g. In fact, the transition is driven by the Bose-Einstein condensation of *real* bosons with $\mathbf{q} = 0$, which occur due to the complete softening of their spectrum at T_c in 3D BFM. Remarkably, the conventional upper critical field, determined as the field, where a non-trivial

solution of the *linearised* Gor'kov equation (19) occurs, is zero in BFM, $H_{c2}(T) = 0$. It is not a finite $H_{c2}(T)$ found in Ref. [17] using MFA. In the homogeneous case $\Delta(T)$ should be determined from Eq.(21) rather than from the BCS-like equation (5), which is actually an identity [12], since $E_0 = -\Sigma_b(0,0)$ below T_c. To get an insight into the magnetic properties of the condensed phase one has to solve Eqs.(6-9, 14-17) and Eq.(21) keeping the nonlinear terms. Even at temperatures well below T_c the condensed state is fundamentally different from the MFA ground state, because of the pairing of bosons. The latter is similar to the Cooper-like pairing of supracondensate ^4He atoms [27], proposed as an explanation of the small density of the single-particle Bose condensate in superfluid Helium-4. The pair-boson condensate should significantly modify the thermodynamic properties of the condensed BFM compared with the MFA predictions. The common wisdom that at weak coupling the boson-fermion model is adequately described by the BCS theory, is therefore negated by our theory.

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